

Supplementary Table 1

Summary of the models for the subunits of mouse complex I

Subunit	Alternative names	Chain	Total residues	Modeled residues	% Modeled	Notes
NDUFV1	51 kDa, Nqo1, NuoF	F	444	10-437	96.4	FMN, 4Fe4S
NDUFV2	24 kDa, Nqo2, NuoE	E	217	5-216	97.7	2Fe2S
NDUFS1	75 kDa, Nqo3, NuoG	G	704	6-693	97.7	2Fe2S, 2 x 4Fe4S
NDUFS2	49 kDa, Nqo4, NuoCD	D	430	1-430	100	Dimethyl-Arg85. No sidechains 40-42 Deactive: 52-60 absent
NDUFS3	30 kDa, Nqo5, NuoCD	C	228	8-213	90.4	
NDUFS7	PSST, Nqo6, NuoB	B	189	35-189	82.0	4Fe4S
NDUFS8	TYKY, Nqo9, Nuol	I	178	1-178	100	No side-chains 8-14, 2 x 4Fe4S
ND1	Nqo8, NuoH	H	318	1-318	100	N-formyl. Deactive: 204-215 absent
ND2	Nqo14, NuoN	N	345	1-344	99.7	N-formyl
ND3	Nqo7, NuoA	A	115	1-115	100	N-formyl. Deactive: 28-48 absent
ND4	Nqo13, NuoM	M	459	1-459	100	N-formyl
ND4L	Nqo11, NuoK	K	98	1-98	100	N-formyl
ND5	Nqo12, NuoL	L	607	1-606	99.8	N-formyl
ND6	Nqo10, NuoJ	J	172	1-171	99.4	N-formyl Deactive: no sidechains 84-118
NDUFV3	10 kDa	s	69	29-68	58.0	
NDUFS4	18 kDa	Q	133	9-133	94.0	
NDUFS5	15 kDa	e	105	1-104	99.0	2 x Cys-Cys
NDUFS6	13 kDa	R	96	1-95	99.0	Zn ²⁺
NDUFA1	MWFE	a	70	1-67	95.7	
NDUFA2	B8	S	98	13-95	84.7	
NDUFA3	B9	b	83	1-83	100	N-acetyl
NDUFA5	B13	V	115	4-115	97.4	
NDUFA6	B14	W	130	17-130	87.7	
NDUFA7	B14.5a	r	112	1-76, 90-122	89.3	N-acetyl
NDUFA8	PGIV	X	171	1-171	100	4 x Cys-Cys
NDUFA9	39 kDa	P	342	1-342	100	Deactive: 186-196, 251-278, 324-335 absent, NADPH
NDUFA10	42 kDa	O	320	1-320	100	ADP
NDUFA11	B14.7	Y	140	1-140	100	Cys-Cys
NDUFA12	B17.2	q	145	1-144	99.3	N-acetyl
NDUFA13	B16.6	Z	143	5-143	97.2	
NDUFAB1 α	SDAP α	T	88	8-82	85.2	4'-phosphopantethine + 3-hydroxyundecanoate
NDUFAB1 β	SDAP β	U	88	1-88	100	4'-phosphopantethine + 3-hydroxydodecanoate
NDUFB1	MNLL	f	56	4-54	91.1	
NDUFB2	AGGG	j	72	6-65	83.3	
NDUFB3	B12	k	103	20-91	69.9	
NDUFB4	B15	m	128	5-128	96.9	
NDUFB5	SGDH	h	143	6-142	95.8	
NDUFB6	B17	i	127	1-35, 62-127	79.5	N-acetyl. No sidechains 62-65, 124-126. 36-61 absent
NDUFB7	B18	o	136	12-116	77.2	2 x Cys-Cys
NDUFB8	ASHI	l	157	3-154	96.8	
NDUFB9	B22	n	178	1-176	98.9	
NDUFB10	PDSW	p	175	2-171	97.1	2 x Cys-Cys
NDUFB11	ESSS	g	122	21-121	82.7	
NDUFC1	KFYI	c	49	2-48	95.9	
NDUFC2	B14.5b	d	120	1-119	99.2	

Supplementary Table 2

The interfaces between subunits in the 3.3 Å structure of mouse complex I

Subunit	Surface area (Å ²)			Local Resolution (Å)	Subunit contacts in order of decreasing contact area	
	Total	Buried	%		Core subunits	Supernumerary subunits
NDUFV1	18,800	6,100	33	3.8 ± 0.3	NDUFV2, NDUFS1	NDUFV3, NDUFS4, NDUFA7
NDUFV2	13,600	4,900	36	3.9 ± 0.3	NDUFV1, NDUFS1	NDUFV3, NDUFS4, NDUFS6
NDUFS1	28,500	10,100	35	3.6 ± 0.3	NDUFV1, NDUFS2, NDUFV2, NDUFS3, NDUFS8	NDUFS4, NDUFA2, NDUFA12, NDUFA6, NDUFA7, NDUFS6, NDUFA9, NDUFV3
NDUFS1 (small)	12,200	7,100	58	3.5 ± 0.2	(NDUFS1 large), NDUFV1, NDUFS2, NDUFV2, NDUFS3, NDUFS8	NDUFS4, NDUFA7, NDUFS6, NDUFA12, NDUFV3
NDUFS1 (large)	19,100	5,600	30	3.7 ± 0.3	NDUFS1 (small), NDUFS3, NDUFS8	NDUFA2, NDUFS4, NDUFA12, NDUFA6, NDUFA9, NDUFV3
NDUFS2	21,300	14,400	68	3.4 ± 0.1	NDUFS3, NDUFS8, NDUFS7, ND1, ND2, NDUFS1, ND3, ND4, ND4L, ND5	NDUFA7, NDUFA13, NDUFA10, NDUFA5, NDUFS6, NDUFB11, NDUFA6, NDUFS4, NDUFA12
NDUFS3	14,500	10,200	70	3.4 ± 0.1	NDUFS2, NDUFS7, NDUFS1, NDUFS8, ND3	NDUFA5, NDUFS4, NDUFA7, NDUFA6, NDUFA9
NDUFS7	9,000	6,300	70	3.4 ± 0.2	NDUFS2, ND1, NDUFS8, NDUFS3, ND3	NDUFA9, NDUFA12, NDUFA6, NDUFA7, NDUFS4
NDUFS8	13,100	9,600	73	3.4 ± 0.2	NDUFS2, NDUFS7, ND1, NDUFS1, NDUFS3	NDUFA12, NDUFS6, NDUFA7, NDUFA13, NDUFA3, NDUFS4, NDUFA1, NDUFA9, NDUFA5
ND1	16,000	10,700	67	3.5 ± 0.1	ND3, NDUFS7, NDUFS2, ND6, NDUFS8	NDUFA1, NDUFA13, NDUFA3, NDUFA8, NDUFA9, NDUFA12, NDUFA7
ND2	15,200	9,800	65	3.5 ± 0.1	ND4L, ND4, ND5, NDUFS2, ND6, ND3	NDUFA10, NDUFC2, NDUFS5, NDUFA11, NDUFB5, NDUFA8, NDUFB11
ND3	11,000	7,400	67	3.5 ± 0.1	ND1, ND6, NDUFS2, NDUFS7, ND4L, ND2, NDUFS3	NDUFA3, NDUFA6, NDUFA9, NDUFA13, NDUFS5, NDUFA1
ND4	18,200	11,000	60	3.4 ± 0.1	ND5, ND2, NDUFS2	NDUFB11, NDUFB4, NDUFB5, NDUFB1, NDUFB10, NDUFB8, NDUFB9, NDUFA8, NDUFC2, NDUFA11, NDUFA10
ND4L	7,000	5,700	83	3.5 ± 0.1	ND6, ND2, ND5, ND3, NDUFS2	NDUFS5
ND5	28,600	13,900	49	3.6 ± 0.1	ND4, ND2, ND4L, NDUFS2	NDUFB8, NDUFB2, NDUFB9, NDUFB10, NDUFB6, NDUFB4, NDUFB7, NDUFB3, NDUFA11, NDUFAB1β, NDUFB5, NDUFB11
ND6	13,000	8,300	64	3.6 ± 0.2	ND4L, ND3, ND1, ND2	NDUFA13, NDUFS5, NDUFA1, NDUFA9, NDUFA3, NDUFA6
NDUFS4	10,800	6,500	60	3.4 ± 0.1	NDUFS1, NDUFS3, NDUFV1, NDUFS8, NDUFV2, NDUFS2, NDUFS7	NDUFA6, NDUFA9, NDUFV3, NDUFA12, NDUFS6, NDUFA5
NDUFS5	9,600	5,400	56	3.8 ± 0.4	ND2, ND6, ND4L, ND3	NDUFA13, NDUFB5, NDUFA8, NDUFC2, NDUFA1, NDUFA3
NDUFS6	7,500	3,000	40	3.6 ± 0.2	NDUFS8, NDUFS1, NDUFS2, NDUFV2	NDUFA9, NDUFA12, NDUFS4
NDUFA1	6,200	3,700	60	3.6 ± 0.2	ND1, ND6, NDUFS8, ND3	NDUFA8, NDUFA13, NDUFS5, NDUFA7, NDUFA12
NDUFA2	5,500	1,400	25	4.0 ± 0.2	NDUFS1	-
NDUFA3	8,100	3,300	41	3.9 ± 0.3	ND1, ND3, NDUFS8	NDUFA8, NDUFA13, NDUFS5, ND6, NDUFB5
NDUFA5	8,500	2,900	34	3.7 ± 0.2	NDUFS3, NDUFS2, NDUFS8	NDUFA7, NDUFA10, NDUFS4, NDUFA6
NDUFA6	9,300	4,500	48	3.5 ± 0.1	NDUFS3, NDUFS1, ND3, NDUFS2, NDUFS7, ND6	NDUFAB1α, NDUFS4, NDUFA9, NDUFA5
NDUFA7	11,500	6,000	52	3.6 ± 0.2	NDUFS2, NDUFS3, NDUFS8, NDUFS1, NDUFV1, ND1, NDUFS7	NDUFA12, NDUFA13, NDUFA5, NDUFA1
NDUFA8	14,100	6,500	46	3.9 ± 0.2	ND2, ND4, ND1	NDUFA13, NDUFA3, NDUFA1, NDUFC2, NDUFB5, NDUFS5, NDUFC1, NDUFB1
NDUFA9	17,000	4,100	24	3.7 ± 0.3	NDUFS7, NDUFS3, ND1, ND3, NDUFS1, ND6, NDUFS8	NDUFS6, NDUFA6, NDUFS4, NDUFA12
NDUFA10	17,000	3,900	23	3.7 ± 0.2	ND2, NDUFS2, ND4	NDUFC1, NDUFB11, NDUFC2, NDUFA5

NDUFA11	9,300	1,600	17	3.8 ± 0.2	ND5, ND2, ND4, NDUFS2	NDUFB5, NDUFB4
NDUFA12	11,800	4,600	37	3.6 ± 0.2	NDUFS8, NDUFS1, NDUFS7, ND1, NDUFS2	NDUFS6, NDUFA7, NDUFS4, NDUFA9, NDUFA1
NDUFA13	14,000	8,200	59	3.8 ± 0.3	ND3, NDUFS2, ND1, NDUFS8, ND6	NDUFA1, NDUFA3, NDUFS5, NDUFB5, NDUFA7, NDUFA8
NDUFAB1α	5,400	900	17	4.2 ± 0.4	-	NDUFA6
NDUFAB1β	6,300	3,300	53	3.9 ± 0.3	ND5	NDUFB9, NDUFB3, NDUFB6, NDUFB2, NDUFB8, NDUFB5
NDUFB1	5,600	1,700	31	3.9 ± 0.2	ND4	NDUFB5, NDUFB10, NDUFA8, NDUFC2
NDUFB2	6,700	3,200	48	4.1 ± 0.4	ND5	NDUFB3, NDUFB7, NDUFB1 β , NDUFB8, NDUFB6
NDUFB3	7,000	2,800	39	4.1 ± 0.3	ND5	NDUFB2, NDUFB9, NDUFB1 β
NDUFB4	12,600	5,900	47	3.7 ± 0.2	ND4, ND5	NDUFB8, NDUFB9, NDUFB10, NDUFB11, NDUFC2, NDUFA11
NDUFB5	13,700	7,700	56	3.7 ± 0.2	ND4, ND2, ND5	NDUFB10, NDUFS5, NDUFB11, NDUFC2, NDUFB1, NDUFA8, NDUFB9, NDUFB6, NDUFA11, NDUFA13, NDUFB1 β , NDUFA3
NDUFB6	10,700	5,000	47	4.0 ± 0.3	ND5	NDUFB10, NDUFB9, NDUFB7, NDUFB1 β , NDUFB5, NDUFB2, NDUFB11
NDUFB7	9,500	3,900	41	4.3 ± 0.5	ND5	NDUFB8, NDUFB6, NDUFB2, NDUFB10
NDUFB8	13,200	5,500	42	3.7 ± 0.3	ND5, ND4	NDUFB4, NDUFB7, NDUFB9, NDUFB10, NDUFB1 β , NDUFB2
NDUFB9	15,300	7,100	47	3.9 ± 0.3	ND5, ND4	NDUFB1 β , NDUFB4, NDUFB6, NDUFB3, NDUFB5, NDUFB8, NDUFB11
NDUFB10	15,400	8,000	52	3.8 ± 0.2	ND5, ND4	NDUFB11, NDUFB6, NDUFB5, NDUFC2, NDUFB7, NDUFB4, NDUFB1, NDUFB8
NDUFB11	10,500	5,300	51	3.7 ± 0.2	ND4, NDUFS2, ND5, ND2,	NDUFB10, NDUFB5, NDUFA10, NDUFC2, NDUFB9, NDUFB4, NDUFB6
NDUFC1	5,100	1,500	29	4.0 ± 0.3	-	NDUFC2, NDUFA10, NDUFA8
NDUFC2	10,500	4,900	47	3.7 ± 0.2	ND2, ND4	NDUFC1, NDUFB5, NDUFB10, NDUFA8, NDUFA10, NDUFS5, NDUFB11, NDUFB4, NDUFB1
NDUFV3	4,800	2,600	53	3.9 ± 0.3	NDUFV1, NDUFV2, NDUFS1	NDUFS4

Surface areas of contacts between subunits were calculated using the PDBePISA server (<http://www.ebi.ac.uk/pdbe/pisa/>) and reported to 100 Å² accuracy. Local resolutions were estimated using the Local Resolution function in RELION with default parameters, then UCSF Chimera was used to extract the resolution at each atomic coordinate in each subunit and the values were averaged.

Supplementary Table 3

Phospholipids modeled in the structure of active mouse complex I

Phospholipid in mouse	Confidence	Side	Location	Human PDB (5XTD)	Ovine PDB (5LNK)	Porcine PDB (5GUP)
H-401 3PE	1	IMS	Interface of ND1, ND3-TMH1 and ND6 (also loops of NDUFA1 and NDUFA13 in IMS).	PE	PE	PE
H-402 PC1	2	Matrix	Interface of ND1 and ND6 (also loops in C-terminal domain of NDUFA9).	-	-	-
A-201 3PE	2	Matrix	Interface of ND4L and ND6 (also C-terminal TMH of ND5).	-	-	-
N-401 3PE	2	Matrix	Interface of ND2, NDUFA11 and transverse and final TMH of ND5.	CDL	-	CDL
M-501 3PE	1	Matrix	Interface of ND2, ND4 and ND5 transverse helix (also N-terminus of NDUFS2). See also M-502.	PE	-	PE
M-502 3PE	2	IMS	Interface of ND2, ND4 and NDUFA11. See also M501.	PE	-	PE
L-701 3PE	1	Matrix	Interface of ND4 and ND5 and ND5 transverse helix (also loops and TMH of NDUFB8).	PE	-	PE
L-702 CDL	1	Matrix	Interface of ND4, ND5 and NDUFB5 (also NDUFB11). See also L-703, M-503, L-704.	CDL	CDL	CDL
L-703 CDL	2	IMS	Interface of ND4, ND5, NDUFB5, NDUFB6 and NDUFB11 (also NDUFB10 on IMS face). See also L-702, M-503, L-704.	CDL	CDL	-
M-503 3PE	1	IMS	Interface of ND4, ND5 and NDUFB11. See also L-702, L-703, L-704.	PC	(CDL)	-
L-704 3PE	1	IMS	Interface of ND5, NDUFB5 and NDUFB6. See also L-702, L-703, M-503.	-	-	-
M-504 3PE	2	IMS	Interface of ND4, NDUFB1 and NDUFB11 (also NDUFB5 on IMS face).	-	-	-
M-505 3PE	2	Matrix	Interface of ND2, ND4 and NDUFC2 (also C-terminal helix of NDUFA10). See also M-506, M-507.	CDL	-	CDL
M-506 3PE	2	Matrix	Interface of ND2, ND4 and NDUFC2 (also NDUFB1 and C-terminal loop of NDUFA10). See also M-505, M-507.		(PE)	
M-507 CDL	1	IMS	Interface of ND2, ND4, NDUFB1 and NDUFC2 (also C-terminus of NDUFA8 on IMS face). See also M-505, M-506.	CDL	PC	CDL
H-403 3PE	1	Matrix	Interface of ND1, NDUFA3 and NDUFA13 (also helix in NDUFS2 and N-terminus of NDUFS8). See also H-404.	PC	PE	PC
H-404 PC1	1	Matrix	Interface of ND1 and NDUFA13 (also helices of NDUFS8 N-terminus and NDUFA7). See also H-403.	-	-	-
H-405 CDL	1	Matrix	Interface of NDUFA1 and helix of NDUFA12 (also ND1, NDUFS8 and NDUFA7).	-	CDL	-
H-406 PC1	2	Matrix	Interface of helices on ND1, NDUFS7 and NDUFA12 (also NDUFS8).	-	-	-
P-401 PC1	2	Matrix	Interface of ND3-TMH1, amphipathic helices on NDUFS7 and loops in ND3, NDUFS7 and NDUFA9.	-	-	-

The phospholipids were assigned on two confidence levels, where 1 is the highest, based on the quality of the density and interactions with nearby residues. Cases in which partial overlap between phospholipids are observed in different structures are indicated with brackets. Interactions of phospholipids with subunits were determined with a 5 Å cut-off.